Exact solutions of the modified Kratzer potential plus ring-shaped potential in the D-dimensional Schrödinger equation by the Nikiforov-Uvarov method

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Abstract

We present analytically the exact energy bound-states solutions of the Schrödinger equation in D-dimensions for a recently proposed modified Kratzer potential plus ring-shaped potential by means of the conventional Nikiforov-Uvarov method. We give a clear recipe of how to obtain an explicit solution to the wave functions in terms of orthogonal polynomials. The results obtained in this work are more general and true for any dimension which can be reduced to the standard forms in three-dimensions given by other works.

Keywords: Energy eigenvalues and eigenfunctions, modified Kratzer potential, ring-shaped potential, non-central potentials, Nikiforov and Uvarov method.

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I. INTRODUCTION

The important task of quantum mechanics is to find the exact bound-states solution of the Schrödinger equation for certain potentials of physical interest. Generally speaking, there are a few main traditional methods to study the exact solutions of quantum systems like the Coulomb, the harmonic oscillator [1,2], the pseudoharmonic [3,4] and the Kratzer [4,5] potentials. Additionally, in order to obtain the bound-states solutions of central potentials, one has to resort to numerical techniques or approximation schemes. For many of the quantum mechanical systems, most popular approximation methods such as shifted $1/N$ expansion [6], perturbation theory [7], path integral solution [8], algebraic methods with the SUSYquantum mechanics method and the idea of shape invariance, further closely with the factorization mrthod [9], exact quantization rule [10,11], the conventional Nikiforov and Uvarov (NU) method [12-25]. Some of these methods have drawbacks in applications. Although some other methods give simple relations for the eigenvalues, however, they lead to a very complicated relations for the eigenfunctions.

The study of exact solutions of the Schrödinger equation for a class of non-central potentials with a vector potential and a non-central scalar potential is of considerable interest in quantum chemistry [26-35]. In recent years, numerous studies [36-40] have been made in analyzing the bound states of an electron in a Coulomb field with simultaneous presence of Aharanov-Bohm (AB) [41] field, and/or a magnetic Dirac monopole [42], and Aharanov-Bohm plus oscillator (ABO) systems. In most of these studies, the eigenvalues and eigenfunctions are obtained by means of seperation of variables in spherical or other orthogonal curvilinear coordinate systems. The path integral for particles moving in non-central potentials is evaluated to derive the energy spectrum of this system analytically [43]. In addition, the idea of SUSY and shape invariance is also used to obtain exact solutions of such non-central but seperable potentials [44]. Very recently, the conventional NU method has been used to give a clear recipe of how to obtain an explicit exact bound-states solutions for the energy eigenvalues and their corresponding wave functions in terms of orthogonal

polynomials for a class of non-central potentials [45].

Recently, Chen and Dong [46] found a new ring-shaped potential and obtained the exact solution of the Schrödinger equation for the Coulomb potential plus this new ring-shaped potential which has possible applications to ring-shaped organic molecules like cyclic polyenes and benzene. Very recently, Cheng and Dai [47], proposed a new potential consisting from the modified Kratzer's potential [48] plus the new proposed ring-shaped potential in [46]. They have presented the energy eigenvalues for this proposed exactly-solvable non-central potential in three dimensional (i.e., $D = 3$)-Schrödinger equation through the NU method. The two quantum systems solved by Refs [46,47] are closely relevant to each other as they deal with a Coulombic field interaction except for a slight change in the angular momentum barrier acts as a repulsive core which is for any arbitrary angular momentum ℓ prevents collapse of the system in any dimensional space due to the slight perturbation to the original angular momentum barrier.

The conventional Nikiforov-Uvarov (NU) method [12], which received much interest, has been introduced for solving Schrödinger equation [13-21], Klein-Gordon [22,23], Dirac [24] and Salpeter [25] equations. We will follow parallel solution to [47] and give a complete exact bound-states solutions and normalized wave functions of the D-dimensional Schrödinger equation with modified Kratzer plus ring-shaped potential, a Coulombic-like potential with an additional centrifugal potential barrier, for any arbitrary ℓ'-states using the conventional Nikiforov-Uvarov method. Our general solution reduces to the standard three-dimensions given by Ref. [47] in the limiting case of $D = 3$.

This work is organized as follows: in section II, we shall briefly introduce the basic concepts of the NU method. Section III is mainly devoted to the exact solution of the Schrödinger equation in D-dimensions for this quantum system by means of the NU method. Finally, the relevant results are discussed in section IV.

II. BASIC CONCEPTS OF THE METHOD

The NU method is based on reducing the second-order differential equation to a generalized equation of hypergeometric type [12]. In this sense, the Schrödinger equation, after employing an appropriate coordinate transformation $s = s(r)$, transforms to the following form:

$$\psi_n''(s) + \frac{\widetilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0, \tag{1}$$

where $\sigma(s)$ and $\widetilde{\sigma}(s)$ are polynomials, at most of second-degree, and $\widetilde{\tau}(s)$ is a first-degree polynomial. Using a wave function, $\psi_n(s)$, of the simple ansatz:

$$\psi_n(s) = \phi_n(s)y_n(s), \tag{2}$$

reduces (1) into an equation of a hypergeometric type

$$\sigma(s)y_n''(s) + \tau(s)y_n'(s) + \lambda y_n(s) = 0, \tag{3}$$

where

$$\sigma(s) = \pi(s)\frac{\phi(s)}{\phi'(s)}, \tag{4}$$

$$\tau(s) = \widetilde{\tau}(s) + 2\pi(s),\ \tau'(s) < 0, \tag{5}$$

and λ is a parameter defined as

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n\,(n-1)}{2}\sigma''(s), \qquad n = 0, 1, 2, ... \tag{6}$$

The polynomial $\tau(s)$ with the parameter s and prime factors show the differentials at first degree be negative. It is worthwhile to note that λ or λ_n are obtained from a particular solution of the form $y(s) = y_n(s)$ which is a polynomial of degree n. Further, the other part $y_n(s)$ of the wave function (2) is the hypergeometric-type function whose polynomial solutions are given by Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} \left[\sigma^n(s)\rho(s)\right], \tag{7}$$

where B_n is the normalization constant and the weight function $\rho(s)$ must satisfy the condition [12]

$$\frac{d}{ds}w(s) = \frac{\tau(s)}{\sigma(s)}w(s),\ w(s) = \sigma(s)\rho(s). \tag{8}$$

The function π and the parameter λ are defined as

$$\pi(s) = \frac{\sigma'(s) - \widetilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \widetilde{\tau}(s)}{2}\right)^2 - \widetilde{\sigma}(s) + k\sigma(s)}, \tag{9}$$

$$\lambda = k + \pi'(s). \tag{10}$$

In principle, since $\pi(s)$ has to be a polynomial of degree at most one, the expression under the square root sign in (9) can be arranged to be the square of a polynomial of first degree [12]. This is possible only if its discriminant is zero. In this case, an equation for k is obtained. After solving this equation, the obtained values of k are substituted in (9). In addition, by comparing equations (6) and (10), we obtain the energy eigenvalues.

III. EXACT SOLUTIONS OF THE QUANTUM SYSTEM WITH THE NU METHOD

A. Seperating variables of the Schrödinger equation

The modified Kratzer potential plus ring-shaped potential in spherical coordinates is defined as [47]

$$V(r,\theta) = D_e\left(\frac{r - r_e}{r}\right)^2 + \beta\frac{\cos^2\theta}{r^2\sin^2\theta}, \tag{11}$$

where β is positive real constant. The potential in (11) introduced by Cheng-Dai [47] reduces to the modified Kratzer potential in the limiting case of $\beta = 0$ [48]. In fact the energy spectrum for this potential can be obtained directly by considering it as special case of the general non-central seperable potentials [45].

Our aim is to derive analytically the energy spectrum for a moving particle in the presence of a potential (11) in a very simple way. The D-dimensional space Schrödinger equation in spherical polar coordinates written for potential (11) takes the form [1,6]

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}-\frac{2\mu\beta}{\hbar^2}\frac{\cos^2\theta}{\sin^2\theta}\right)\right]\psi(r,\theta,\varphi)$$

$$+\left[D_e\left(\frac{r-r_e}{r}\right)^2-E\right]\psi(r,\theta,\varphi)=0, \tag{12}$$

where $\mu=\frac{m_1m_2}{m_1+m_2}$ being the reduced mass of the two particles and $\psi(r,\theta,\varphi)$ being the total wave function separated as follows

$$\psi_{n\ell m}(r,\theta,\varphi)=R(r)Y_\ell^m(\theta,\varphi),\ R(r)=r^{-(D-1)/2}g(r),\ Y_\ell^m(\theta,\varphi)=H(\theta)\Phi(\varphi). \tag{13}$$

On substituting equation (13) into (12) leads to a set of second-order differential equations:

$$\left[\frac{1}{r^{D-1}}\frac{d}{dr}\left(r^{D-1}\frac{d}{dr}\right)-\frac{L_{D-1}^2}{r^2}\right]R(r)+\frac{2\mu}{\hbar^2}\left[E-D_e\left(\frac{r-r_e}{r}\right)^2\right]R(r)=0, \tag{14}$$

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)-\frac{m^2}{\sin^2\theta}-\frac{2\mu\beta}{\hbar^2}\frac{\cos^2\theta}{\sin^2\theta}+\ell(\ell+D-2)\right]H(\theta)=0, \tag{15}$$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2}+m^2\Phi(\varphi)=0, \tag{16}$$

where $L_{D-1}^2=\ell(\ell+D-2)$. The solution in (16) is periodic and must satisfy the period boundary condition $\Phi(\varphi+2\pi)=\Phi(\varphi)$ from which we obtain

$$\Phi_m(\varphi)=\frac{1}{\sqrt{2\pi}}\exp(\pm im\varphi),\quad m=0,1,2,..... \tag{17}$$

Therefore, we are left to solve equations (14) and (15). After lengthy, but straightforward, calculations, Equation (14), representing the radial wave equation can be rewritten as [6]:

$$\frac{d^2g(r)}{dr^2}+\left[\frac{2\mu}{\hbar^2}(E-D_e)+\frac{4\mu D_er_e}{\hbar^2}\frac{1}{r}-\frac{\widetilde{\nu}+(2\mu D_er_e^2/\hbar^2)}{r^2}\right]g(r)=0, \tag{18}$$

where

$$\widetilde{\nu} = \frac{1}{4}(M-1)(M-3),\ M = D + 2\ell. \tag{19}$$

The two particles in equation (18) interacting via Coulombic-like field have a slight change in the angular momentum barrier acts as a repulsive core which for any arbitrary ℓ prevents collapse of the system in any space dimension due to the additional centrifugal potential barrier. On the other hand, equation (15) representing the angular wave equation takes the simple form

$$\frac{d^2H(\theta)}{d\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{dH(\theta)}{d\theta} + \left[\ell(\ell+D-2) - \frac{m^2 + (2\mu\beta/\hbar^2)\cos^2\theta}{\sin^2\theta}\right]H(\theta) = 0. \tag{20}$$

Therefore, equations (18) and (20) have to be solved latter by using the NU method in the following subsections.

B. The solutions of the angular equation

In order to apply NU method, we introduce a new variable $s = \cos\theta$, equation (20) is then rearranged as the universal associated-Legendre differential equation [45,49]

$$\frac{d^2H(s)}{ds^2} - \frac{2s}{1-s^2}\frac{dH(s)}{ds} + \frac{\nu'(1-s^2) - m'^2}{\sin^2\theta}H(\theta) = 0, \tag{21}$$

where

$$\nu' = \ell'(\ell'+D-2) = \ell(\ell+D-2) + 2\mu\beta/\hbar^2 \quad \text{and} \quad m'^2 = m^2 + 2\mu\beta/\hbar^2. \tag{22}$$

The solution of this equation has already been solved by the NU method in [45,47]. However, the aim in this subsection is to solve with different parameters resulting from the D-space-dimensions of Schrödinger equation. Upon letting $D = 3$, we can readily obtain the standard case given in [47]. Equation (21) is compared with (1) and the following identifications are obtained

$$\widetilde{\tau}(s) = -2s, \quad \sigma(s) = 1 - s^2, \quad \widetilde{\sigma}(s) = -\nu' s^2 + \nu' - m'^2. \tag{23}$$

Inserting the above expressions into equation (9), one obtains the following function:

$$\pi(s) = \pm\sqrt{(\nu' - k)s^2 + k - \nu' + m'^2}. \tag{24}$$

Following the method, the polynomial $\pi(s)$ is found in the following possible values

$$\pi(s) = \begin{cases} m's & \text{for } k_1 = \nu' - m'^2, \\ -m's & \text{for } k_1 = \nu' - m'^2, \\ m' & \text{for } k_2 = \nu', \\ -m' & \text{for } k_2 = \nu'. \end{cases} \tag{25}$$

Imposing the condition $\tau'(s) < 0$, for equation (5), one selects

$$k_1 = \nu' - m'^2 \quad \text{and} \quad \pi(s) = -m's, \tag{26}$$

which yields form equation (5)

$$\tau(s) = -2(1 + m')s. \tag{27}$$

Using equations (6) and (10), the following expressions for λ are obtained, respectively,

$$\lambda = \lambda_n = 2n(1 + m') + n(n - 1), \tag{28}$$

$$\lambda = \nu' - m'(1 + m'). \tag{29}$$

We compare equations (28) and (29) and from the definition $\nu' = \ell'(\ell' + D - 2)$, the new angular momentum ℓ' values are obtained as

$$\ell' = -\frac{(D-2)}{2} + \frac{1}{2}\sqrt{(D-2)^2 + 4(n + \sqrt{m^2 + 2\mu\beta/\hbar^2})(n + 1 + \sqrt{m^2 + 2\mu\beta/\hbar^2})}, \tag{30}$$

which can be reduced to the simple form

$$\ell' = n + m', \tag{31}$$

in three-dimensions [47]. Using equations (2)-(4) and (7)-(8), the wave function can be written as,

$$H_{m'}(\theta) = N_{\ell' m'} \sin(\theta)^{m'} P_n^{(m',m')}(\cos\theta), \tag{32}$$

where $N_{\ell' m'} = \sqrt{\frac{(2\ell'+1)(\ell'-m')!}{2(\ell'+m')!}}$ is the normalization constant given in [46,47] and

$$n = -\frac{(1 + 2m')}{2} + \frac{1}{2}\sqrt{(2\ell' + 1)^2 + 4\ell'(D - 3)}, \tag{33}$$

with m' is defined by equation (22).

C. The solutions of the radial equation

The solution of the SE for the modified central Kratzer's potential has already been solved by means of NU-method in [48]. Very recently, using the same method, the problem for the non-central potential in (11) has been solved in three dimensions by Cheng and Dai [47]. However, the aim of this subsection is to solve the problem with a different radial separation function $g(r)$ in any arbitrary dimensions. We now study the bound-states (real) solution $E < D_e$ of equation (18). Letting

$$\varepsilon = \sqrt{-\frac{2\mu}{\hbar^2}(E - D_e)},\ \alpha = \frac{4\mu D_e r_e}{\hbar^2},\ \gamma = \widetilde{\nu} + \frac{1}{2}\alpha r_e, \tag{34}$$

and substituting these expressions in equation (18), one gets

$$\frac{d^2 g(r)}{dr^2} + \left(\frac{-\varepsilon^2 r^2 + \alpha r - \gamma}{r^2}\right) g(r) = 0. \tag{35}$$

To apply the conventional NU-method, equation (35) is compared with (1) and the following expressions are obtained

$$\widetilde{\tau}(r) = 0, \quad \sigma(r) = r, \quad \widetilde{\sigma}(r) = -\varepsilon^2 r^2 + \alpha r - \gamma. \tag{36}$$

Substituting the above expressions into equation (9) gives

$$\pi(r) = \frac{1}{2} \pm \frac{1}{2}\sqrt{4\varepsilon^2 r^2 + 4(k - \alpha)r + 4\gamma + 1}. \tag{37}$$

According to this conventional method, the expression in the square root be the square of a polynomial. Thus, the two roots k can be readily obtained as

$$k = \alpha \pm \varepsilon\sqrt{4\gamma + 1}. \tag{38}$$

In view of that, we arrive at the following four possible functions of $\pi(r)$:

$$\pi(r) = \begin{cases} \frac{1}{2} + \left[\varepsilon r + \frac{1}{2}\sqrt{4\gamma + 1}\right] & \text{for } k_1 = \alpha + \varepsilon\sqrt{4\gamma + 1}, \\ \frac{1}{2} - \left[\varepsilon r + \frac{1}{2}\sqrt{4\gamma + 1}\right] & \text{for } k_1 = \alpha + \varepsilon\sqrt{4\gamma + 1}, \\ \frac{1}{2} + \left[\varepsilon r - \frac{1}{2}\sqrt{4\gamma + 1}\right] & \text{for } k_2 = \alpha - \varepsilon\sqrt{4\gamma + 1}, \\ \frac{1}{2} - \left[\varepsilon r - \frac{1}{2}\sqrt{4\gamma + 1}\right] & \text{for } k_2 = \alpha - \varepsilon\sqrt{4\gamma + 1}. \end{cases} \tag{39}$$

The correct value of $\pi(r)$ is chosen such that the function $\tau(r)$ given by equation (5) will have negative derivative [12]. So we can select the physical values to be

$$k = \alpha - \varepsilon\sqrt{4\gamma+1} \quad \text{and} \quad \pi(r) = \frac{1}{2} - \left[\varepsilon r - \frac{1}{2}\sqrt{4\gamma+1}\right], \tag{40}$$

which yield

$$\tau(r) = -2\varepsilon r + (1 + \sqrt{4\gamma+1}). \tag{41}$$

Using equations (6) and (10), the following expressions for λ are obtained, respectively,

$$\lambda = \lambda_n = 2N\varepsilon, \ N = 0, 1, 2, ..., \tag{42}$$

$$\lambda = \alpha - \varepsilon(1 + \sqrt{4\gamma+1}). \tag{43}$$

So we can obtain the energy eigenvalues as

$$E_N = D_e - \frac{8\mu D_e^2 r_e^2/\hbar^2}{\left(2N + 1 + \sqrt{(M-1)(M-3) + 8\mu D_e r_e^2/\hbar^2 + 1}\right)^2}, \tag{44}$$

where

$$(M-1)(M-3) = 4\widetilde{\nu} = (D-2)^2 + 4\ell'(\ell' + D - 2) - 8\mu\beta/\hbar^2 - 1, \tag{45}$$

with ℓ' defined in (30). Therefore, the final energy spectra in equation (44) take the following Coulombic-like form [7]

$$E_{N'} = D_e - \frac{2\mu D_e^2 r_e^2/\hbar^2}{(N')^2}, \ N' = 0, 1, 2, ... \tag{46}$$

where

$$N' = \frac{1}{2}\left[2N + \sqrt{(D-2)^2 + 4\ell'(\ell' + D - 2) + 8\mu(D_e r_e^2 - \beta)/\hbar^2} + 1\right], \tag{47}$$

is simply obtained by means of substituting equation (45) into (44).

(i) If $D = 3$, equation (44), with the help of equation (45), is transformed into the following form

$$E_{Nnm} = D_e - \frac{8\mu D_e^2 r_e^2/\hbar^2}{\left(2N+1+\sqrt{(2n+1)^2+4m^2+4(2n+1)\sqrt{m^2+2\mu\beta/\hbar^2}+8\mu D_e r_e^2/\hbar^2}\right)^2}, \tag{48}$$

and it is consistent with equation (40) in [47].

(ii) If, $D = 3$ and $\beta = 0$ (modified Kratzer potential), equation (44) is transformed into the form

$$E_n = D_e - \frac{8\mu D_e^2 r_e^2/\hbar^2}{\left(1+2n+\sqrt{1+4\ell(\ell+1)+8\mu D_e r_e^2/\hbar^2}\right)^2}. \tag{49}$$

and it is consistent with equation (14) in [48].

Let us now turn attention to find the radial wavefunctions for this potential. Using $\tau(r)$, $\pi(r)$ and $\sigma(r)$ in equations (4) and (8), we find

$$\phi(r) = r^{(\sqrt{4\gamma+1}+1)/2} e^{-\varepsilon r}, \tag{50}$$

$$\rho(r) = r^{\sqrt{4\gamma+1}} e^{-2\varepsilon r}. \tag{51}$$

Then from equation (7), we obtain

$$y_n(r) = B_n r^{-\sqrt{4\gamma+1}} e^{2\varepsilon r} \frac{d^N}{dr^N}\left(r^{N+\sqrt{4\gamma+1}} e^{-2\varepsilon r}\right), \tag{52}$$

and the wave function $g(r)$ can be written in the form of the generalized Laguerre polynomials as

$$g(r) = C_{N,L} r^{L+1} e^{-\varepsilon r} L_N^{2L+1}(2\varepsilon r), \tag{53}$$

where L can be found easily from equation (47). Finally, the radial wave functions of the Schrödinger equation are obtained

$$R(r) = C_{N,L} r^{L-(D-3)/2} e^{-\varepsilon r} L_N^{2L+1}(2\varepsilon r), \tag{54}$$

where

$$\varepsilon = \frac{\mu a}{\hbar^2 N'} \tag{55}$$

with N' is given in equation (47) and $C_{N,L}$ is the normalization constant to be determined below. Using the normalization condition, $\int_0^\infty R^2(r) r^{D-1} dr = 1$, and the orthogonality relation of the generalized Laguerre polynomials, $\int_0^\infty z^{\eta+1} e^{-z} \left[L_n^\eta(z)\right]^2 dz = \frac{(2n+\eta+1)(n+\eta)!}{n!}$, we have

$$C_{N,L} = \sqrt{\frac{(2\varepsilon)^{2L+3} N!}{2(N+L+1)(N+2L+1)!}}. \tag{56}$$

Therefore, we may express the normalized total wave functions as

$$\psi(r,\theta,\varphi) = \sqrt{\frac{(2\varepsilon)^{2L+3}(2\ell'+1)(\ell'-m')!N!}{4\pi(\ell'+m')!(N+L+1)(N+2L+1)!}} r^{L-(D-3)/2} \exp(-\varepsilon r) L_N^{2L+1}(2\varepsilon r)$$

$$\times \sin(\theta)^{m'} P_n^{(m',m')}(\cos\theta) \exp(\pm i m\varphi). \tag{57}$$

IV. RESULTS AND CONCLUSIONS

In this paper, the Schrödinger equation in any arbitrary dimensions has been solved for its exact bound-states with a recently proposed modified Kratzer potential plus ring-shaped potential by means of a simple conventional NU method. The analytical expressions for the total energy levels of this system is found to be different from the results obtained for the modified Kratzer's potential in [48] and also more general than the one obtained recently in three-dimensions [47]. Therefore, the noncentral potentials treated in [45] can be introduced as perturbation to the modified Kratzer's potential by adjusting the strength of the coupling constant β in terms of D_e, which is the coupling constant of the modified Kratzer's potential. In addition, the angular part, the radial part and then the total wave functions are also found. Thus, the Schrödinger equation with a new non-central but separable potential has also been studied (cf. [45] and the references therein). This method is very simple and useful in solving other complicated systems analytically without given a restiction conditions on the solution of some quantum systems as the case in the other models. Finally, we point out

that these exact results obtained for this new proposed form of the potential (11) may have some interesting applications in the study of different quantum mechanical systems, atomic and molecular physics.

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